

Renormalization group contraction of tensor networks in three dimensions

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We present a new strategy for contracting tensor networks in arbitrary geometries. This method is designed to follow as strictly as possible the renormalization group philosophy, by first contracting tensors in an exact way and, then, performing a controlled truncation of the resulting tensor. We benchmark this approximation procedure in two dimensions against an exact contraction. We then apply the same idea to a three dimensional system. The underlying rational for emphasizing the exact coarse graining renormalization group step prior to truncation is related to monogamy of entanglement.

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Computing analytically the properties of a quantum model is, in general, not possible. It is then necessary to resort to classical simulations that rely on approximation techniques. From a quantum information perspective, the presence of a small amount of entanglement in the system has been identified as the key ingredient that allows for efficient classical simulations. This has been exploited in one dimension (1D) in a series of algorithms based on a description of the system as a tensor network. Following this approach, condensed matter systems can be simulated using Matrix Product States (MPS, [1, 2]) as the testbed for the variational procedure of the density-matrix renormalization group (DMRG, [3]) to study ground states of local 1D Hamiltonians. Beyond the 1D setting, the computation of physical magnitudes using tensor networks is limited by the numerical effort necessary to perform the contraction of the tensor network, *i.e.* to sum all its indices. The efficiency for performing this task is limited by the area law scaling of the entanglement entropy in the system [4–7]. To overcome this problem, several strategies aim at finding the best possible approximation to the contraction of tensor networks after identifying the relevant degrees of freedom of the system [8–10].

Let us briefly recall the key elements of the tensor network representation. Given a quantum state of N particles $|\psi\rangle = \sum c^{i_1, \dots, i_N} |i_1 \dots i_N\rangle$ its coefficients can be represented as a contraction of local tensors $c^{i_1, \dots, i_N} = \text{tr}(A^{1, i_1} \dots A^{N, i_N})$, where each local tensor A^j carries a physical index i_j and ancillary indices (which are not written) that get contracted according to a prescribed geometry. The rank of these ancillary indices, that we shall call χ , controls the amount of entanglement which is captured by the tensor representation. If the tensors are simple matrices on a line, the tensor network is called MPS [1, 2]. Other possible geometries are regular squared grids in any dimensions that correspond to PEPS [11], and tree-like structures that go under the name of TTN [12] and MERA [13].

In this letter we propose a new strategy to contract tensor networks in general geometries, that we shall il-

lustrate in detail for PEPS in 2D and 3D. The method is based on following as strictly as possible the renormalization group (RG) philosophy. First, an exact contraction of a set of local tensors is performed that produces a coarse grained tensor of larger rank. Subsequent contractions would make the rank of the effective tensors to scale following a law dictated by the geometry of the tensor network. For instance, in the case of PEPS the rank of the coarse grained tensors would grow following an area law. It is then necessary to perform a truncation that faithfully retains only relevant degrees of freedom. To achieve this truncation, our method makes a series of Schmidt decompositions that cast the relevant information onto a renormalized tensor.

The strategy we present here differs from a previous renormalization group inspired proposal [14–16]. There, the original tensor is first truncated and then contracted efficiently. Instead, we first contract exactly tensors at a larger numerical cost, and then truncate. This procedure can be made exact in 1D [17]. In more dimensions, this idea entails a trade off between numerical computation speed and precision. Our proposal relies on the idea that in higher dimensions, *e.g.* 3D, monogamy of entanglement makes every degree of freedom to have a reduced amount of entanglement with each neighbor. Long distance correlations emerge from the multiplicity of possible paths connecting local degrees of freedom. Therefore, a tensor network with small rank χ is already a good approximation to a 3D system. The fact that good tensor network representations only need a small χ makes viable our proposal for exact contractions followed by truncation.

Let us recall that, in 2D settings, some variants of contraction schemes for PEPS have been analyzed [11, 14–16]. To our knowledge, PEPS renormalization methods have not been applied to 3D systems, which nevertheless have been studied using cluster states [18] or string bond states [19]. For 3D classical systems other renormalization algorithm have been proposed [20, 21].

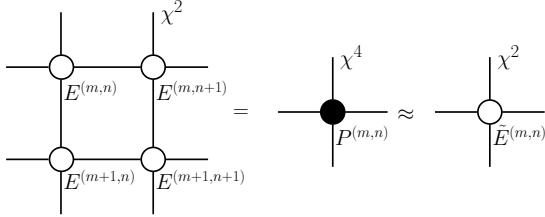
RG contraction in 2D.— Let us illustrate our method for contraction of tensor networks with the computa-

tion of the norm of a state in 2D. We start by considering the norm of the original state $|\psi\rangle$, that is the folded lattice made of tensors of the form $E^{(m,n)} = \sum_i A^{*(m,n)i} \otimes A^{(m,n)i}$, where (m, n) labels a position in the 2D lattice and physical indices i at this point have been summed over. Each tensor $E^{(m,n)}$ has four further ancillary indices of rank χ^2 (not written explicitly) pointing to its 2D neighbors. The global contraction of the 2D tensor network corresponds to the computation of the norm $\langle\psi|\psi\rangle = \text{Tr}(E^{(1,1)} \dots E^{(N,N)})$, where Tr is a generalized trace that contracts all ancillary indices.

The stages in our contraction strategy go schematically as follows. We start with the tensor $E^{(m,n)}$ which carries 4 indices of rank χ^2 . We first contract four adjacent tensors to build a plaquette $P^{(m,n)} = E^{(m,n)} E^{(m,n+1)} E^{(m+1,n)} E^{(m+1,n+1)}$. Now $P^{(m,n)}$ carries a total of 8 open indices of rank χ^2 , showing the area law increase of indices naturally associated to the contraction of tensors in a 2D square lattice. This plaquette tensor will be approximated by a renormalized tensor on a coarse grained lattice $\tilde{E}^{(m,n)} \approx P^{(m,n)}$, where we shall truncate to a tensor of 4 indices of rank χ^2 . The global contraction symbolically reads

$$\langle\psi|\psi\rangle = \text{Tr}(\{E\}) = \text{Tr}(\{P\}) \approx \text{Tr}(\{\tilde{E}\}), \quad (1)$$

which can be graphically represented as



where tensors E are represented by nodes connected to its neighboring tensors with lines that represent ancillary indices. After a renormalization step, we recover the same lattice structure with renormalized tensors.

Let us now discuss in more detail each step in the renormalization group contraction we have just sketched. Though computationally expensive, the initial exact contraction $\{E\} \rightarrow \{P\}$ has two main advantages. First, an exact contraction of the tensors in a plaquette retains all degrees of freedom, making this method specially suitable for systems with frustration at the plaquette scale. Furthermore, by an appropriate renormalization of the virtual bonds of the P tensors we recover the original lattice structure, modulo an increase in the rank of ancillary indices. When completing the strategy with a truncation, it will then be possible to perform a systematic iteration of the same procedure, resulting in the global contraction of the tensor network. The method is thus a way to escape from the area law restriction at the cost of a truncation of the renormalized tensors.

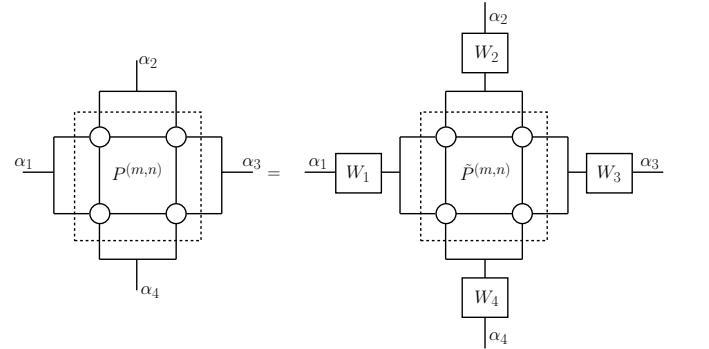
Once we have constructed the renormalized tensor $P^{(m,n)}$, we need to perform a controlled truncation. Let us modify the notation to make this step clearer, by dropping the site label and introducing explicitly the ancillary indices $P^{(m,n)} = P_{\alpha_1 \alpha_2 \alpha_3 \alpha_4}$. Each ancillary index α is the result of combining the two ancillary indices that were attached to tensors E pointing towards an adjacent plaquette. To be concrete, we call α_1 the index connecting the plaquette to its upper neighbor. This index is the combination of two indices from the original tensors $\alpha_1 = \beta_1 \otimes \beta'_1$. Thus, each α is a combined index of rank χ^4 . We then select the index α_1 and separate it from the rest of indices of the plaquette by means of a singular value decomposition

$$P_{\alpha_1 \alpha_2 \alpha_3 \alpha_4} = U_{\alpha_1 \mu} \lambda^\mu V_{\mu \alpha_2 \alpha_3 \alpha_4} \quad (2)$$

where U and V are unitary matrices and λ^μ are the eigenvalues in the decomposition. It is convenient to include the squared root of the eigenvalues into the unitary matrix $U_{\alpha_1 \mu}$ as follows

$$W_{\alpha \mu} = U_{\alpha \mu} \sqrt{\lambda^\mu}. \quad (3)$$

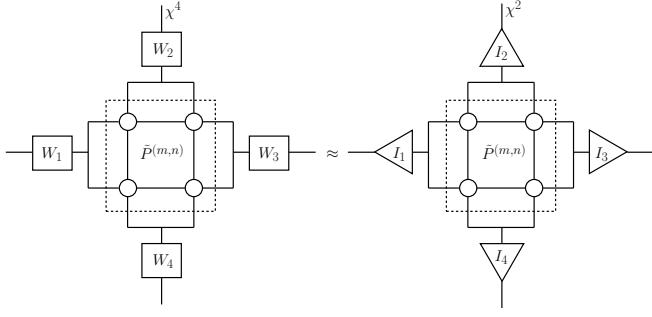
We repeat this process for each index in order to obtain the four matrices W_1, W_2, W_3 and W_4 as follows



After these four successive decompositions, we can construct a new tensor $\tilde{P} = W_1^{-1} W_2^{-1} W_3^{-1} W_4^{-1} P$, where we have used pseudo inverse matrices.

We proceed now to perform a renormalization of the plaquette P using the set of tensors W s. The key observation here is that, along each direction, the plaquette is surrounded by other plaquettes decomposed in a similar way. We assume that a plaquette $P = W_1 W_2 W_3 W_4 \tilde{P}$ has neighboring unitaries W'_1, W'_2, W'_3 and W'_4 . The renormalization consists on the truncation of the degrees of freedom between plaquettes through the unitaries W and W' . We first take matrices W_1 and W'_3 to form tensor $R_{3,1} = W'_3 W_1$ which can be decomposed using a SVD into $R_{3,1} = \tilde{U} \Sigma \tilde{V}$. The truncation corresponds to only keeping the largest χ^2 eigenvalues from matrix Σ to generate the new decomposition $R_{3,1} \approx I_3 I_1$, where each matrix I is the projection to W onto the relevant eigenvalue subspace. We repeat this procedure for each neighboring

pair W and W' . We then apply the four matrices I_k to \tilde{P} to obtain our final truncation $\tilde{E} = I_1 I_2 I_3 I_4 \tilde{P}$



This truncation strategy that delivers the renormalized tensor \tilde{E} can be represented as

$$P = \text{Tr}(EEEE) = W_1 W_2 W_3 W_4 \tilde{P} \approx I_1 I_2 I_3 I_4 \tilde{P} = \tilde{E}$$

and reduces the size of the plaquette tensor to χ^2 for each bond.

The procedure described above is computationally demanding compared to variational methods or other renormalization techniques. In order to make the singular value decomposition in Eq. 2 it is necessary to make the contraction of a plaquette with its own adjoint

to obtain each of the W_k . This strategy outperforms the naive use of singular value decomposition algorithms.

As mentioned above, previous proposals for the renormalization of tensors networks rely on a decomposition of the local tensors before producing a truncation [14–16]. Such a decomposition allows to achieve a higher bond dimension after the original truncation. Other approaches work with square plaquettes that include the physical indices [22]. It is also important to notice that the method proposed here is not a variational procedure, though it remains numerically stable.

Validation in 2D.— We validate our approach showing results for the renormalization of a tensor network representing the ground state of the Ising Hamiltonian with a transverse magnetic field in a square lattice

$$H = - \sum_{\{i,j\}} \sigma_i^z \sigma_j^z + h \sum_i \sigma_i^x. \quad (5)$$

where $\{i,j\}$ are neighboring sites on finite or infinite lattices. This model displays a phase transition at a critical field $h_c \approx 3.04$ for the infinite square lattice.

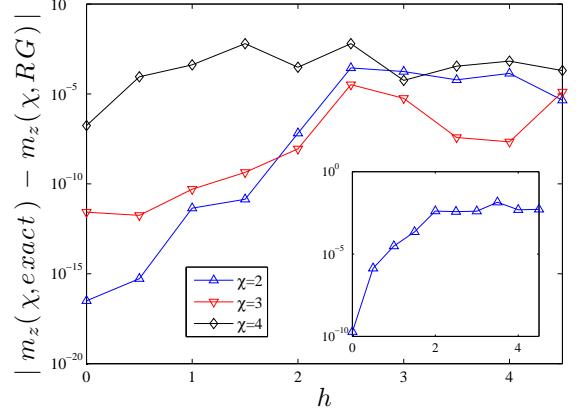


FIG. 1. For an Ising model with transverse field in a finite 2D square lattice of size 6×6 , we plot the error of the magnetization between the exact contraction and our renormalization group contraction of the same PEPS, that is $|m_z(\chi, \text{exact}) - m_z(\chi, RG)|$, for different values of χ . Inset: Same for a 12×12 lattice with $\chi = 2$.

The preparation of the tensor network can be performed using an imaginary time evolution [11, 23], $|\psi_f\rangle = e^{-Ht}|\psi_0\rangle$. We first proceed to use a Trotter approximation to this Euclidean evolution. At each step we have to apply the evolution operator T to a pair of neighboring tensors $\Theta_{\alpha,\beta}^{i',j'} = T_{i,j}^{i',j'} [A_{\alpha,\mu}^i]_k [A_{\mu,\beta}^j]_{k+1}$ and truncate the new tensors $[A_{\alpha,\mu}^i]_k$ and $[A_{\mu,\beta}^j]_{k+1}$ to the lattice bond dimension.

In order to validate our strategy, we show in Fig.1 the error of the magnetization m_z in a finite square lattice of size 6×6 and 12×12 , with our RG contraction against the exact contraction of the very same tensors, that is $|m_z(\chi, \text{exact}) - m_z(\chi, RG)|$. The error introduced by the RG contraction is of the order of 10^{-3} at the critical point. Let us note that this error is smaller for $\chi = 2$ since the RG casts χ^{16} numbers to χ^8 . It is thus expected that the faithfulness of RG is better for small χ . Obviously, the $\chi = 4$ tensor is in itself a better representation of the state.

3D quantum systems.— The contraction strategy for tensor networks we have presented in 2D can be extended for a 3D square lattice. The renormalization is performed over plaquettes of eight tensors forming a cube. We use a singular value decomposition to decouple at each step four ancillary indices, and obtain the unitaries corresponding to each orthogonal direction. This set of six matrices W_k is combined with unitaries W'_k associated to neighboring plaquettes, to produce six truncated matrices I_k . We perform a similar operation along each direction to recover the renormalized tensors with bond dimension χ^2 . To overcome limitations in computational resources, we use an operation similar to the trick in 4 and obtain each of the unitaries W_i . For a single direc-

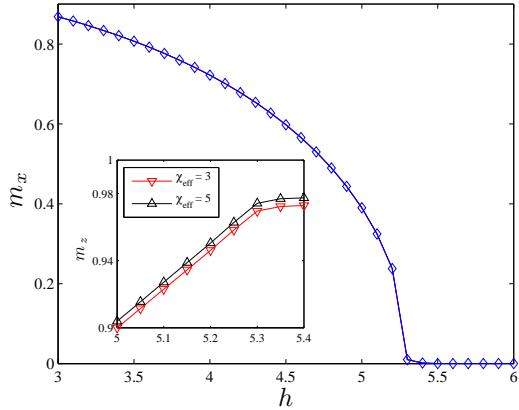
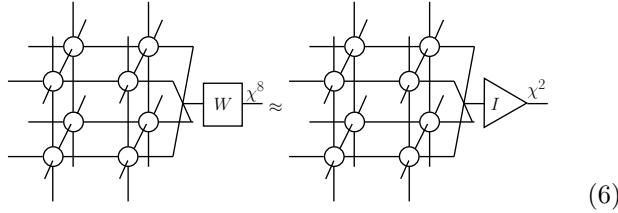


FIG. 2. Magnetization m_z vs. local field h for the Ising model with transverse field in an infinite 3D square lattice. The critical point is found at $h_c \approx 5.29$. The rank of the tensor network is $\chi = 2$. Inset: Magnetization m_x vs. h for different values of χ_{eff} .

tion, this renormalization is represented as



It is possible to prepare the original state with a tensor network using some specific χ . Yet, after a first contraction is made, we can retain renormalized tensors with a larger effective χ_{eff} . We have checked that for $\chi = 2$, stable results are obtained for $\chi_{\text{eff}} \sim 5$.

We can now apply our approach to 3D systems to compute the magnetization of Ising model Eq.5 for an infinite 3D square lattice, by iterating the above procedure. The state is prepared using a minimal environment to stabilize the Trotter evolution. The results for the magnetizations m_z and m_x for $\chi = 2$ are presented in Fig.2. A quantum phase transition is detected at a critical point located around $h_c \simeq 5.29$ (series expansions detect a critical point at $h_c = 5.14$ [24]). We have also computed the equivalent phase transition in 2D, using again only $\chi = 2$ tensors. In the 2D case, our RG contraction finds a transition at $h_c \simeq 3.25$ to be compared with the result $h_c = 3.04$ coming from other more precise methods. This hints at the fact that RG contraction is a better approximation in 3D than in 2D.

Conclusions.— We have presented a novel, RG inspired strategy to contract tensor networks that delivers good results in a 3D simulation of the phase transition in the quantum Ising model. Our scheme can be extended to hexagonal and triangular lattices, where a renormalization step can be performed choosing the plaquettes to

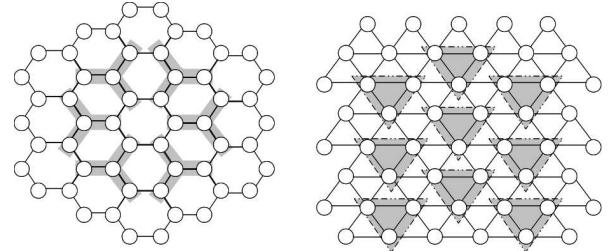


FIG. 3. Renormalization of hexagonal and triangular lattices, forming plaquettes with the tensors inside the shaded areas.

be contracted as in Fig.3 so as to recover a rescaled version of the original lattice. This opens the possibility of studying frustrated models in 3D using PEPS technology.

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